

# The thermal denaturation of Peyrard-Bishop model with an external potential

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**Abstract.** The impact of various types of external potentials to the Peyrard-Bishop DNA denaturation is investigated through statistical mechanics approach. The partition function is obtained using transfer integral method, and further the stretching of hydrogen bond is calculated using time independent perturbation method. It is shown that all types of external potentials accelerate the denaturation processes at lower temperature. In particular, it is argued that the Gaussian potential with infinitesimal width reproduces a constant force at one end of DNA sequence as already done in some previous works.

PACS numbers: 87.14.gk, 87.15.ad, 87.15.A-

## 1. Introduction

It has been known that the base-pairs of double-helix break up and dissociate from each other to form two separated random coils when a solution of DNA macromolecules is heated up to 80°C. This phenomenon is referred as the DNA denaturation or the thermal DNA melting ([1] and references therein). On the other hand, at lower temperature before melting two strands of DNA can also be separated by applying an oppositely directed force on two strands at the DNA terminal point. This is known as the force-induced DNA melting [1]. Theoretically, the phenomena have been discussed in many works, for instance the work by Hanke *et.al.* on the denaturation of stretched DNA [2]. Also using the worm-like chain, the opened double-stranded DNA can be explained by a force exceeding certain critical value [3, 4]. On the other hand, the study of shear effect of pulling force shows that the shear unzipping of a heteropolymer would be similar to the unzipping in a tensile mode with sequence heterogeneity [5, 6].

It has been shown that a random external force would drastically change the phase diagram, while the ground state develops bubbles with various lengths as the random force fluctuation is increased. The fluctuating force denaturates the DNA by a gradual increase of bubble sizes. This suggests the possibility of opening up local bubbles in the selective regions without breaking the whole DNA [7]. The denaturation at lower temperature is realized by the enzymes, protein and so forth [8]. The effects are influenced by many factors such as the alkaline compound filling up a cell. Some works also investigated another effects, for instance the phase transition in a short DNA using the Peyrard-Bishop (PB) with additional delta function potential [9]. The paper argued that the denaturation is a localization-delocalization transition process. In the case without any external force, the denaturation is a second order transition, while under an external force it becomes the first-order one [1]. Following the same line, the present paper deals with external potentials interacting to DNA within the PB model, and investigates its effects to the denaturation process.

This paper is organized as follows. First of all the PB model with various external potentials is briefly introduced. It is then followed with the statistical mechanics formulation on the partition function of Hamiltonian under consideration. Before ending the paper with summary, the detail calculation of hydrogen bond stretching using first order time independent perturbation and its thermal behavior are presented in Secs. 3 and 4.

## 2. The Model

Following the original PB model, the motion of DNA molecules is represented by transversal displacement,  $u_n$  and  $v_n$ , corresponding to the base displacement from their equilibrium position along the direction of hydrogen bonds that is represented by the Morse potential to connect two bases in a pair [10].

The paper adopts the PB model with an additional external potential  $V$  which has

the same direction as Morse potential,

$$H = \sum_n \frac{1}{2M} \dot{u}_n^2 + \frac{\kappa}{2} (u_n - u_{n-1})^2 + \sum_n \frac{1}{2M} \dot{v}_n^2 + \frac{\kappa}{2} (v_n - v_{n-1})^2 + \frac{D}{2} \left( e^{-\frac{\alpha}{2}\sqrt{2}(u_n - v_n)} - 1 \right)^2 + V(u_n - v_n). \quad (1)$$

Performing a transformation to the center of mass coordinate representing the in-phase and out-phase transversal motions, one can define  $X_n = (u_n + v_n)/\sqrt{2}$  and  $Y_n = (u_n - v_n)/\sqrt{2}$ . Then, it yields the PB Hamiltonian [10],

$$H = \sum_n \frac{1}{2M} p_n^2 + \frac{\kappa}{2} (X_{n+1} - X_n)^2 + \sum_n \frac{1}{2M} P_n^2 + \frac{\kappa}{2} (Y_{n+1} - Y_n)^2 + \frac{D}{2} (e^{-\alpha/2 Y_n} - 1)^2 + V(Y_n), \quad (2)$$

where  $D$  and  $\alpha$  are the depth and inverse width of the potential respectively.  $p_n = M\dot{X}_n$ ,  $P_n = M\dot{Y}_n$  and  $\kappa$  is the spring constant.

It should be remarked that some previous works suggested that the  $n$ -th nucleotide in one strand might preferably interacts with the  $(n \pm h)$ -th nucleotides in another strand with  $h = 4$  or  $5$  [11, 12, 13]. However for the sake of simplicity, throughout the paper let us consider the original PB model with taking into account only the nearest neighbor nucleotides of another strand. The extension to the cases of  $h \neq 1$  should require extensive numerical studies that is out of our current interest. The variable  $X_n$  is decoupled from  $Y_n$  corresponding merely to the linear chain, while  $Y_n$  represents the stretching motion that is our main interest. So, from now let us ignore the  $X_n$  part in further calculation.

### 3. Mechanical statistics calculation

Now let us calculate the mechanical statistics behavior of current system using transfer integral method. Having certain hamiltonian of an equilibrium system, one can extract some physical observables through statistical mechanics approach. The approach is particularly suitable to investigate the dynamics of DNA with thermal fluctuations since the exact solution of its equation of motion never exists [14]. Within the PB model, the DNA denaturation and its melting temperature have previously been studied in term of temperature [10, 12]. It was argued that the denaturation can be induced by energy localization due to nonlinear effects, and also should be highly influenced by external interactions like  $V_n$  in the present case.

Using the hamiltonian in Eq. (2), one can consider the partition function to further calculate some thermodynamics variables. In [10, 14], the calculation has been performed using transfer integral method for  $V = 0$ . This paper follows the same procedure. In the canonical ensemble the partition function density is related to the Hamiltonian by  $Z \propto \exp(\beta H)$ . For the present case it reads,

$$Z = \int \int \prod_{n=1}^N \prod_{n=0}^N dP_n dY_n \exp \left\{ -\beta \left[ \sum_n \frac{P_n^2}{2M} + \frac{\kappa}{2} (Y_n - Y_{n-1})^2 \right] \right\}$$

$$+\frac{D}{2} \left( e^{-\alpha/2 Y_n} - 1 \right)^2 + V(Y_n) \Big] \Big\} \delta(Y_N - Y_0) , \quad (3)$$

where  $\beta = 1/kT$  with  $k$  is the Boltzmann constant. It can further be decomposed into its momentum and coordinate spaces,  $Z = Z_P Z_Y$  with,

$$Z_P = \int \prod_{n=1}^N dP_n \exp \left( -\beta \sum_n \frac{P_n^2}{2M} \right) , \quad (4)$$

$$Z_Y = \int \prod_{n=0}^N dY_n \delta(Y_N - Y_0) \exp \left\{ -\beta \left[ \frac{\kappa}{2} (Y_n - Y_{n-1})^2 + \frac{D}{2} (e^{-\alpha/2 Y_n} - 1)^2 + V(Y_n) \right] \right\} , \quad (5)$$

The Gaussian integration in Eq. (4) yields,

$$Z_P = \left( \sqrt{\frac{2\pi M}{\beta}} \right)^N . \quad (6)$$

On the other hand, Eq. (5) reads,

$$Z_Y = \int \prod_{n=0}^N dY_n \delta(Y_N - Y_0) \prod_{n=1}^N e^{-\beta \Theta(Y_n, Y_{n-1})} , \quad (7)$$

where,

$$\Theta(Y_n, Y_{n-1}) = \frac{\kappa}{2} (Y_n - Y_{n-1})^2 + \frac{D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1)^2 + V(Y_n) . \quad (8)$$

This can be solved using transfer integral method.

Shifting the operator  $Y_{n-1} \rightarrow Y_n$  and defining an eigenfunction  $\phi(Y_n)$  that satisfies [14],

$$\int dY_{n-1} e^{-\beta \Theta(Y_n, Y_{n-1})} \phi_i(Y_{n-1}) = e^{-\beta E_i} \phi_i(Y_n) , \quad (9)$$

Eq. (7) becomes,

$$Z_Y = \int \prod_{n=0}^N dY_n \delta(Y_N - Y_0) e^{-\beta E_i} \phi_i(Y_n) . \quad (10)$$

Since  $\delta(Y_N - Y_0) = \sum_i \phi_i^*(Y_N) \phi_i(Y_0)$  and taking the normalization  $\int dY \phi^* \phi = 1$ , one gets,

$$Z_Y = \sum_i e^{-\beta N E_i} . \quad (11)$$

Let us find the eigenfunction  $\phi(y)$  and the eigenvalue  $E$  of Eq.(9). First of all at continuum limit,  $Y_{n-1} \sim x$  and  $Y_n \sim y$ , Eq. (9) reads,

$$\int dx \phi(x) \exp \left\{ -\beta \left[ \frac{\kappa}{2} (y - x)^2 + \frac{D}{2} (e^{-\alpha/2 y} - 1)^2 + V(y) \right] \right\} = e^{-\beta E} \phi(y) . \quad (12)$$

Now assuming that the harmonic term is dominant,  $x = y + z$  can be expanded as a Taylor series in the power of  $z$ . The expansion up to the second order yields,

$$\begin{aligned} & \int dz e^{-\frac{\beta\kappa}{2}z^2} \left[ \phi(y) + \frac{d\phi}{dy}z + \frac{1}{2}\frac{d^2\phi}{dy^2}z^2 \right] \\ &= \exp \left\{ -\beta \left[ E - \frac{D}{2} (e^{-\alpha/2 y} - 1)^2 + V(y) \right] \right\} \phi(y) . \end{aligned} \quad (13)$$

Again, this is just the Gaussian integration and the result is [15],

$$\begin{aligned} \phi(y) + \frac{1}{2\beta\kappa} \frac{d^2\phi}{dy^2} &= \exp \left\{ -\beta \left[ E + \frac{1}{2\beta} \ln \left( \frac{2\pi}{\beta\kappa} \right) \right. \right. \\ &\quad \left. \left. - \frac{D}{2} (e^{-\frac{\alpha}{2}y} - 1)^2 + V(y) \right] \right\} \phi(y) \\ &\approx \left[ 1 - \beta E - \frac{1}{2} \ln \left( \frac{2\pi}{\beta\kappa} \right) \right] \phi(y) \\ &\quad + \beta \left[ \frac{D}{2} (e^{-\alpha/2 y} - 1)^2 + V(y) \right] \phi(y) . \end{aligned} \quad (14)$$

This is nothing else than the Schrödinger like equation,

$$-\frac{1}{2m_0} \frac{d^2\phi}{dy^2} + \frac{D}{2} [e^{-\alpha/2 y} - 1]^2 \phi + V(y)\phi = \bar{E}\phi , \quad (15)$$

where  $m_0 = \kappa\beta^2$  and  $\bar{E} = E + 1/(2\beta) \ln [2\pi/(\beta\kappa)]$ . The problem is therefore turned into finding the eigenvalue of Eq. (15).

Eq. (15) then yields an eigen equation  $H\phi_m = \bar{E}_m\phi_m$  with Hamiltonian,

$$H = \frac{1}{2m_0} \frac{d^2}{dy^2} + \frac{D}{2} [e^{-\alpha/2 y} - 1]^2 + V(y) , \quad (16)$$

and  $m$  is an integer. For a constant force  $V_0$ ,  $V(y) = V_0 y$ , the transformation  $\phi = \exp(\beta V_0 y)\psi$  reproduces the Schrödinger equation with Morse potential [16]. Unfortunately, the equation can be solved only for few special cases. Generally, the solution can be obtained perturbatively by assuming that the potential  $V(y)$  is small enough compared to the Morse potential. Under this assumption, the eigen equation can be solved using time independent perturbation theory in standard quantum mechanics. However, it should be emphasized that the problem remains a classical one, and the quantum mechanics is borrowed only for technical reason since the calculation yields the Schrödinger equation.

In quantum mechanics the perturbation is applied by expanding the Hamiltonian ( $H$ ) in a form of  $H = H_0 + \epsilon V$  with  $H_0$  is the hamiltonian in Eq. (16) without the potential, while  $\epsilon$  is a small parameter. According to the time-independent perturbation theory, the eigenvalue and its eigenfunction can be written as [17],

$$\bar{E}_m = \bar{E}_m^{(0)} + \epsilon \bar{E}_m^{(1)} + \epsilon^2 \bar{E}_m^{(2)} + \dots , \quad (17)$$

$$\phi_m(y) = \phi_m^{(0)}(y) + \epsilon \phi_m^{(1)}(y) + \epsilon^2 \phi_m^{(2)}(y) + \dots . \quad (18)$$

The eigenvalue for  $H_0$  is determined by  $H_0\phi^{(0)} = \bar{E}_0^{(0)}\phi^{(0)}$ , that is,

$$-\frac{1}{2m_0} \frac{d^2\phi^{(0)}}{dy^2} + \frac{D}{2} (e^{-\alpha/2 y} - 1)^2 \phi^{(0)} = \bar{E}^{(0)}\phi^{(0)} , \quad (19)$$

where  $\bar{E}^{(0)} = E^{(0)} + 1/(2\beta) \ln[2\pi/(\beta\kappa)]$ . The equation is just the well known Schrödinger equation with Morse potential and the solution has been derived in [14]. Substituting  $y' = (1/2)\alpha y$ ,  $\lambda = 2\sqrt{m_0 D}/\alpha$ ,  $\mathcal{E}^{(0)} = 8m_0/\alpha^2 \bar{E}^{(0)}$  and  $z = 2\lambda \exp(-y')$ , one arrives at the eigenvalue problem for  $\beta\sqrt{\kappa D}/\alpha > 1/2$  as [18, 17],

$$-\frac{d^2\phi^{(0)}}{dy'^2} + \lambda^2 \left( e^{-2y'} - 2e^{-y'} \right) \phi_m^{(0)} = \mathcal{E}_m^{(0)} \phi_m^{(0)}. \quad (20)$$

The eigenvalue and its eigenfunction are,

$$\mathcal{E}_m^{(0)} = - \left( \lambda - m - \frac{1}{2} \right)^2, \quad (21)$$

$$\phi_m^{(0)} = N_m z^{b_m} e^{-z/2} L_m^{2b_m}(z), \quad (22)$$

where  $b_m = \lambda - m - 1/2$  and  $N_m = m! [\Gamma(m+1) \Gamma(2\lambda - m)]^{-1/2}$  with  $\Gamma$  is the Gamma function.  $L_m^{2b_m}(z) = (z^{-2b_m} e^z / m!) (d^m(e^{-z} z^{m+2b_m}) / dz^m)$  is the associated Laguerre polynomial or generalized Laguerre polynomials.

Based on these transformation, using the standard procedure in quantum mechanics one obtains the solution up to the first order [17],

$$\mathcal{E}_m = \mathcal{E}_m^{(0)} + \epsilon \mathcal{E}_m^{(1)}, \quad (23)$$

$$\phi_m(y') = \phi_m^{(0)}(y') + \epsilon \phi_m^{(1)}(y'), \quad (24)$$

where,

$$\mathcal{E}_m^{(1)} = \int dy' \phi_m^{(0)*}(y') V(y') \phi_m^{(0)}(y'), \quad (25)$$

$$\phi_m^{(1)}(y') = \sum_{k \neq m} \frac{\int dy' \phi_k^{(0)*}(y') V(y') \phi_m^{(0)}(y')}{\mathcal{E}_m^{(0)} - \mathcal{E}_k^{(0)}} \phi_k^{(0)}(y'). \quad (26)$$

Finally the partition function of  $y$  is given by,

$$Z_y = \sum_m e^{-\beta N E_m}, \quad (27)$$

with the eigenvalue,

$$E_m = \frac{\alpha^2}{8\kappa\beta^2} \mathcal{E}_m + \frac{1}{2\beta} \ln \left( \frac{\beta\kappa}{2\pi} \right). \quad (28)$$

#### 4. Thermal denaturation

One of relevant parameters in the study of DNA denaturation is the mean stretching,  $\langle y_n \rangle$ , of the hydrogen bond. It is defined as,

$$\langle y_n \rangle = \frac{1}{Z} \int dy_n dp_n \prod_{n=1}^N y_n e^{-\beta H}. \quad (29)$$

The average value of hydrogen bond stretching can be calculated through,

$$\langle y \rangle = \frac{\sum_{i=1}^N \langle \phi_i(y) | y | \phi_i(y) \rangle e^{-N\beta \bar{E}_i}}{\sum_{i=1}^N \langle \phi_i(y) | \phi_i(y) \rangle e^{-N\beta \bar{E}_i}}. \quad (30)$$

At the limit of large  $N$ ,  $\langle y \rangle$  is dominated by the ground state [14], that is  $\langle y \rangle = \int dy (\phi_0(y))^* y \phi_0(y)$ . Up to the leading term of perturbation, *i.e.*  $\phi_0(y) = \phi_0^{(0)}(y) + \epsilon \phi_0^{(1)}(y)$ , Eq. (30) reads,

$$\begin{aligned} \langle y \rangle &= \int dy \phi_0^{(0)*}(y) y \phi_0^{(0)}(y) \\ &+ \epsilon \left[ \int dy \phi_0^{(0)*}(y) y \phi_0^{(1)}(y) + \int dy \phi_0^{(1)*}(y) y \phi_0^{(0)}(y) \right]. \end{aligned} \quad (31)$$

The higher order of eigenvalue and eigenfunction are given by,

$$\mathcal{E}_0^{(1)} = \int dy \phi_0^{(0)*}(y) V(y) \phi_0^{(0)}(y), \quad (32)$$

and,

$$\begin{aligned} \phi_0^{(1)}(y) &= \sum_{k \neq 0} \frac{\int dy \phi_k^{(0)*} V(y) y \phi_0^{(0)}(y)}{\mathcal{E}_0^{(0)} - \mathcal{E}_k^{(0)}} \phi_k^{(0)}(y), \\ &= \frac{\int dy \phi_1^{(0)*} V(y) \phi_0^{(0)}(y)}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}} \phi_1^{(0)}(y) + \frac{\int dy \phi_2^{(0)*} V(y) \phi_0^{(0)}(y)}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}} \phi_2^{(0)}(y) + \dots \end{aligned} \quad (33)$$

Then Eqs. (22)~(26) yield,

$$\begin{aligned} \langle y \rangle &= I_{(00)} + \epsilon \left[ \frac{I_{(10)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}} \int dy \phi_0^{(0)*}(y) y \phi_1^{(0)}(y) \right. \\ &+ \frac{I_{(10)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}} \int dy \phi_1^{(0)*}(y) y \phi_0^{(0)}(y) \\ &+ \frac{I_{(20)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}} \int dy \phi_0^{(0)*}(y) y \phi_2^{(0)}(y) \\ &\left. + \frac{I_{(20)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}} \int dy \phi_2^{(0)*}(y) y \phi_0^{(0)}(y) + \dots \right] + O(\epsilon^2), \end{aligned} \quad (34)$$

where,

$$I_{00} = \int dy \phi_0^{(0)*}(y) V(y) \phi_0^{(0)}(y), \quad (35)$$

$$I_{10} = \int dy \phi_1^{(0)*}(y) V(y) \phi_0^{(0)}(y), \quad (36)$$

$$I_{20} = \int dy \phi_2^{(0)*}(y) V(y) \phi_0^{(0)}(y), \quad (37)$$

while the eigenvalues and eigenfunctions are given by,

$$\mathcal{E}_0^{(0)} = - \left( \lambda - \frac{1}{2} \right)^2, \quad (38)$$

$$\mathcal{E}_1^{(0)} = - \left( \lambda - \frac{3}{2} \right)^2, \quad (39)$$

$$\mathcal{E}_2^{(0)} = - \left( \lambda - \frac{5}{2} \right)^2. \quad (40)$$

...

Here,

$$\phi_0^{(0)} = \frac{(2\lambda)^{\lambda-1/2}}{\sqrt{\Gamma(2\lambda)}} e^{-\lambda \exp(-\alpha/2 y)} e^{-\alpha/2(\lambda-1/2)y}, \quad (41)$$

$$\begin{aligned} \phi_1^{(0)} &= \frac{2(2\lambda)^{\lambda-\frac{3}{2}}}{\sqrt{\Gamma(2)\Gamma(2\lambda-1)}} e^{-\lambda \exp(-\alpha/2 y)} e^{-\alpha/2(\lambda-3/2)y} \\ &\times [-\lambda e^{-\alpha/2 y} + (\lambda-1)], \end{aligned} \quad (42)$$

$$\begin{aligned} \phi_2^{(0)} &= \frac{4(2\lambda)^{\lambda-5/2}}{\sqrt{\Gamma(3)\Gamma(2\lambda-2)}} e^{-\lambda \exp(-\alpha/2 y)} e^{-\alpha/2(\lambda-5/2)y} \\ &\times \left[ \lambda^2 e^{-\alpha y} - \lambda(2\lambda-3) e^{-\alpha/2 y} + \frac{1}{4}(2\lambda-3)(2\lambda-4) \right], \end{aligned} \quad (43)$$

where  $\lambda = 2\sqrt{\kappa D}/(\alpha k_B T)$ .

Considering the case of linear potential  $V(y) = V_0 y$ , the wave function is given by,

$$\phi_0(y) = \phi_0^{(0)} + \epsilon \left[ \frac{V_0 \int dy \phi_1^{(0)*} y \phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}} \phi_1^{(0)}(y) + \frac{V_0 \int dy \phi_2^{(0)*} y \phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}} \phi_2^{(0)}(y) + \dots \right]. \quad (44)$$

The variation of wave function in respect to temperature is depicted in Fig. 1 for the same parameters as [12], that is  $D = 0.04$  eV,  $\alpha = 4.45$  Å<sup>-1</sup>,  $\epsilon = 0.01$ ,  $\kappa = 0.06$  eV/Å<sup>2</sup> and  $V_0 = 15$  pN.

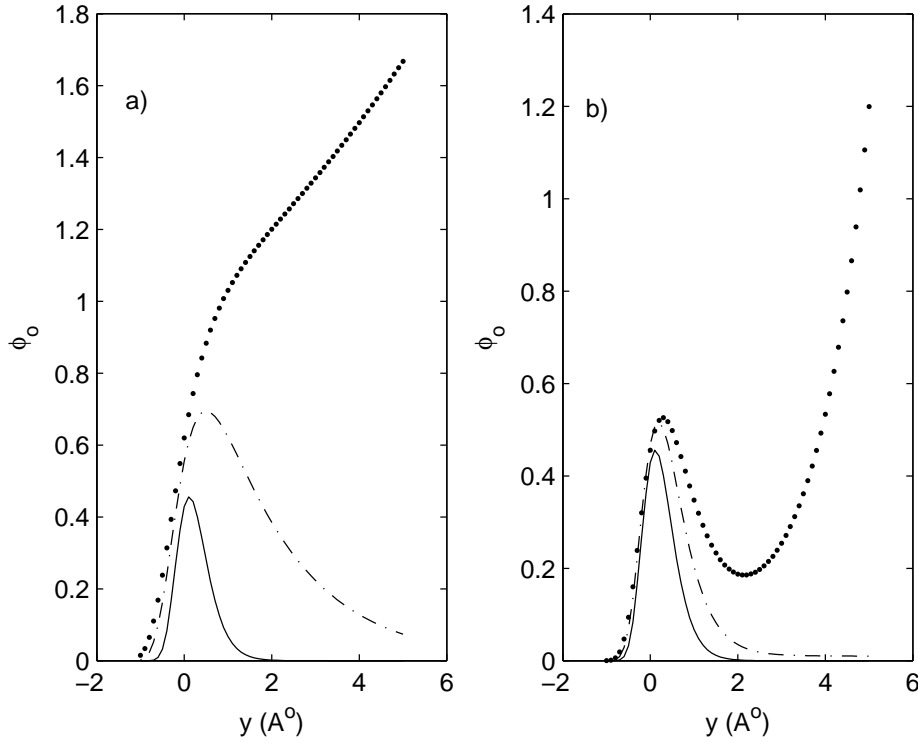
The ground state of eigenfunction for linear potential gives the weighting factor for the calculation of DNA displacement  $\langle y \rangle$  [10]. The figure shows that at low temperature, the peak is close to the minimum of Morse potential and decays exponentially as the displacement increases. Without the external potential, the eigenfunction is increasing drastically at the melting temperature, that is about 500K as already pointed out in [12]. On the other hand, the same behavior occurs at lower temperature when the external potential is applied to the system, *i.e.* at about 200K.

From Eq. (34), the influence of various external potentials into denaturation processes is depicted in Fig. 2 using the same parameters as [12]. The figure describes the effects of linear potential  $V(y) = V_0 y$ , sinusoidal potential  $V(y) = V_0 \sin(ay)$  and Gaussian potential  $V(y) = V_0 e^{-ay^2}$  with  $a$  is a constant. It should be noted that the result coincides to the previous work for zero external potential [12]. The figure shows that the critical temperature is approximately around 400K without external potential, and around 200K with constant external potential. Nevertheless the critical temperature becomes around 350K for periodic sinusoidal force with  $a = 2.5$ . The same behavior of  $\langle y \rangle$  for non forcing condition has also been obtained in [19] using flexible chain model with typical parameter  $D = 0.25$  eV,  $\alpha = 2.8$  Å<sup>-1</sup> and numerical calculation of the stochastic description of flexible polymer models.

## 5. Summary

The effect of external potential to the Peyrard-Bishop DNA denaturation has been investigated for various types of potential : linear potential  $V(y) = V_0 y$ , sinusoidal





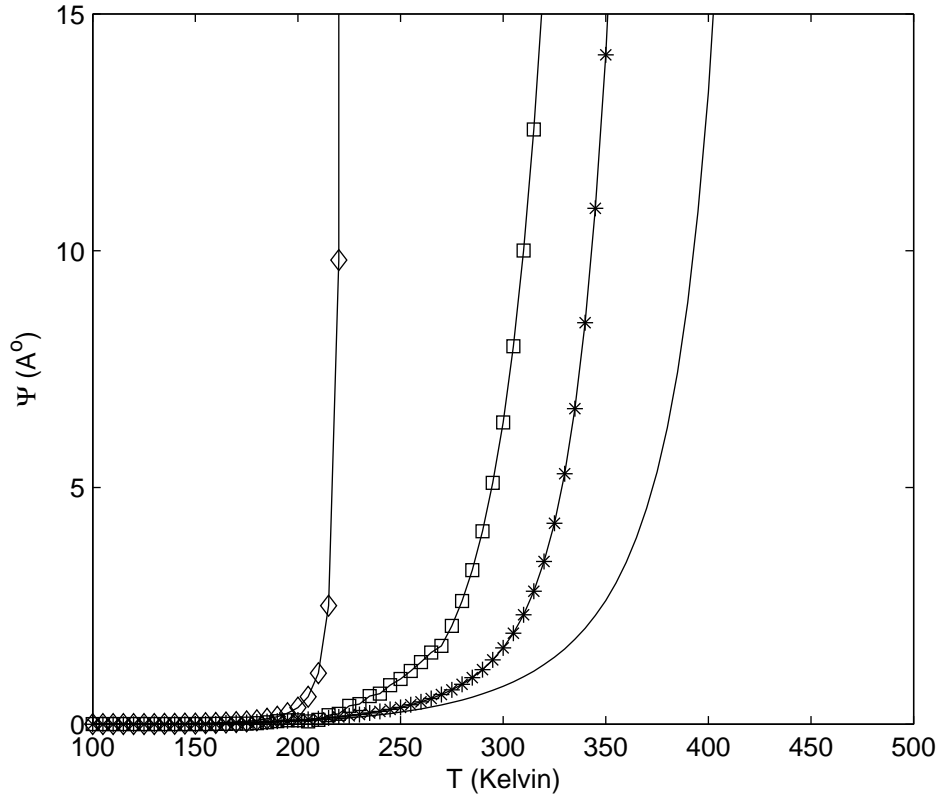
**Figure 1.** The eigenfunction without (left) and with (right) external linear potential as a function of the displacement in various temperatures : 100K (solid line), 300K (dashed-line) and 500K (dotted-line) in the left; and 100K (solid line), 150K (dashed-line) and 200K (dotted-line) in the right figures.

potential  $V(y) = V_0 \sin(ay)$  and Gaussian potential  $V(y) = V_0 e^{-ay^2}$  with  $a$  is a constant. The DNA denaturation and its melting temperature have further been studied in the framework of statistical mechanics approach. The calculation of partition function has been performed perturbatively using transfer integral method to obtain analytically the mean stretching of hydrogen bond.

The present paper support the results of previous works. In a cell, DNA strands can be separated by applying certain external potential [20], or in chemical terms by enzymes whose interactions with DNA could make the strand separation thermodynamically favorable at ambient temperature [21]. It has been shown that two strands of double-stranded DNA can be separated by applying  $V_0 \sim 15$  pN force at room temperature. The model also predicts that the DNA overstretching force should be a decreasing function of temperature, or in another word the melting temperature should be a decreasing function of the applied force [20, 22].

## Acknowledgments

AS thanks the Group for Theoretical and Computational Physics LIPI for warm hospitality during the work. This work is funded by the Indonesia Ministry of Research



**Figure 2.** The hydrogen bond stretching as a function of melting temperature using the same parameters as [12] for various potentials :  $V(y) = 0$  (plain line),  $V(y) = V_0 y$  (line with diamonds),  $V(y) = V_0 \sin(2.5y)$  (line with squares) and  $V(y) = V_0 e^{-10y^2}$  (line with stars) .

and Technology and the Riset Kompetitif LIPI in fiscal year 2011 under Contract no. 11.04/SK/KPPI/II/2011. FPZ thanks Research KK ITB 2012 and Hibah Kompetensi Kemendikbud RI 2012.

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